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Introduction

In small, heavy water moderated reactors, the critical mass depends strongly on the fast neutron leakage which, in turn, is quite sensitive to the slowing down model used (see Figure 1). Since the two-group method is restricted to a Yukawa slowing down kernel and D_2O is better represented by an age-Yukawa kernel, an harmonics method for systems with spherical symmetry was investigated to check its suitability for making critical mass calculations for the HRT.

This method is an extension of the harmonics method discussed by Schweinler[1] and Goertzel and Garabedian[2] to include the calculation of reactors having multiplication in the reflector. Although the method is limited to reactors in which the slowing down properties are independent of position, resonance capture, the amount of which is different in the core and reflector, can be included by the usual artifice of first calculating the slowing down density without resonance capture and then multiplying with the resonance escape probability to obtain the source of thermal neutrons. Functions representing neutron fluxes, absorptions, productions and thermalizations are expanded in harmonic functions which vanish at the outer boundary of the total reactor system. Since an infinite order determinant must vanish to satisfy the criticality condition, the convergence of the sub-determinants becomes important for practical calculations.

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1. Schweinler, H. C., Mon-P-152.

2. Goertzel, G. and Garabedian, H. L., ORNL-30.

ORNL-LR-DWG-303

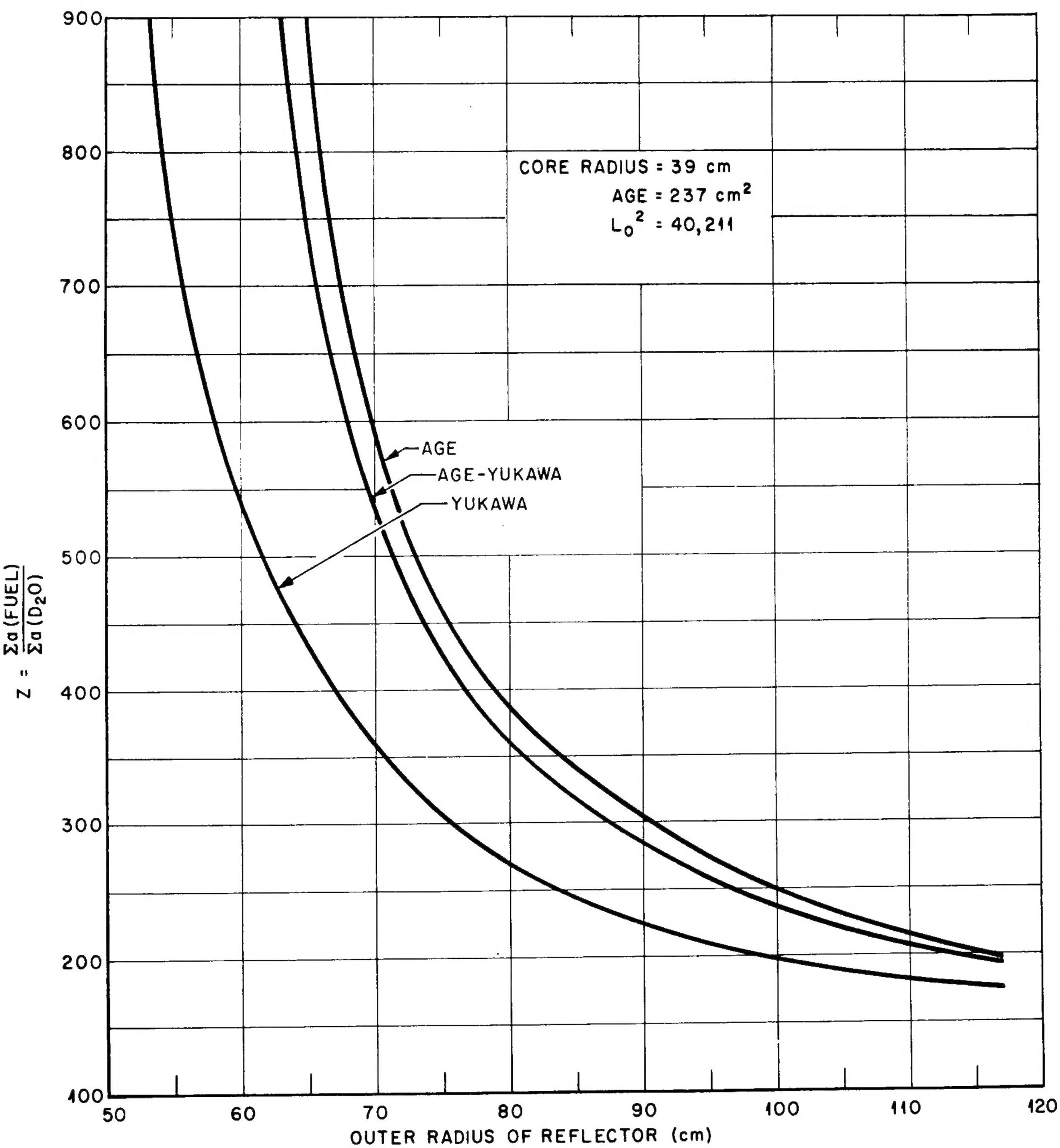

Fig. 1. Comparison of Different Slowing Down Kernels in D_2O

In particular, an attempt is made to set limitations on the applicability of a second order determinant by comparison with closed form two-group results.

It is found that for reactors of HRT size, the method converges very rapidly and for all practical purposes, the critical condition is well represented by the vanishing of a second order determinant which leads, not to a transcendental equation, but merely a second degree algebraic equation for the critical concentration of fuel in the core. In general, the harmonics method, as will be apparent from the development which is given below, converges more rapidly the smaller the ratio of reflector thickness to core radius. On the other hand, it has been observed that the rate of convergence also depends on the outer radius of the reflector; the smaller is the overall size of the reactor, the more rapid the convergence.

Derivation of Harmonics Method

The derivation of this method closely follows CF-51-5-98[3], with the exception that resonance escape probabilities are allowed to be different in core and reflector and resonance capture is assumed to take place just above thermal energies. The reactor equations applicable to the entire reactor can be written in the following form in which Σ_a and k are considered to be functions of position;

$$D\nabla^2\phi(\underline{r}) - \Sigma_a(\underline{r})\,\phi(\underline{r}) + q(\underline{r}) = 0 \tag{1}$$

$$q(\underline{r})/p(\underline{r}) = \int_{\text{Reactor}} k(\underline{r}')\,\Sigma_a(\underline{r}')\,P(\underline{r},\underline{r}')\,dr' \tag{2}$$

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3. Weinberg, A. M. and Noderer, L. C., "Theory of Neutron Chain Reactions," Volume II, Part I.

where D = thermal diffusion coefficient

ϕ = thermal neutron flux

Σ_a = thermal absorption cross section

q = thermal slowing down density

p = resonance escape probability

k = fast neutrons produced per thermal absorption

$P(\underline{r}, \underline{r}')$ = finite slowing down kernel (normalized to unity).

For a reflected reactor it is assumed that P and D are the same in reflector and core. Orthonormal functions $Z_i(\underline{r})$ which vanish at the extrapolated boundary and satisfy the wave equation,

$$\nabla^2 Z_i(\underline{r}) + B_i^2 Z_i(\underline{r}) = 0 \tag{3}$$

are used to expand the following functions:

$$\phi(\underline{r}) = \sum_i C_i Z_i(\underline{r}) \tag{4}$$

$$\Sigma_a(\underline{r})\phi(\underline{r}) = \sum_i G_i Z_i(\underline{r}) \tag{5}$$

$$k(\underline{r})\Sigma_a(\underline{r})\phi(\underline{r}) = \sum_i E_i Z_i(\underline{r}) \tag{6}$$

$$q(\underline{r})/p(\underline{r}) = \sum_i A_i Z_i(\underline{r}) \tag{7}$$

$$q(\underline{r}) = \sum_i H_i Z_i(\underline{r}) \tag{8}$$

By applying the orthonormality relations, it is possible to express E_i and G_i in terms in the C's as follows;

$$G_i = \sum_j (\Sigma_{ac}\lambda_{ij} + \Sigma_{ab}\nu_{ij})\, C_j \tag{9}$$

$$E_i = \sum_j (k_c\Sigma_{ac}\lambda_{ij} + k_b\Sigma_{ab}\nu_{ib})\, C_j \tag{10}$$

where

$$\lambda_{ij} = \int_{\text{Core}} Z_i(\underline{r})\, Z_j(\underline{r})\, \underline{dr} \tag{11}$$

$$\nu_{ij} = \int_{\text{Reflector}} Z_i(\underline{r})\, Z_j(\underline{r})\, \underline{dr} \tag{12}$$

and subscripts c and b refer to core and reflector (blanket) respectively.

Since equations (6) and (10) define the analytic continuation of $k\Sigma_a\phi$ over all space equation (2) can be rewritten

$$\begin{aligned} q/p &= \sum_i E_i \int_{\text{Reactor}} Z_i(\underline{r}')P(\underline{r}, \underline{r}')\, \underline{dr}' \\ &= \sum_i E_i \int_{\substack{\text{all}\\ \text{space}}} Z_i(\underline{r}')P_\infty(/\underline{r} - \underline{r}'/)\, \underline{dr}' \\ &= \sum_i E_i\overline{P_\infty}\,(B_i^2)\, Z(\underline{r}) \end{aligned} \tag{13}$$

where $P_\infty(/\underline{r} - \underline{r}'/)$ is the slowing down kernel evaluated at thermal energy in an infinite medium and $\overline{P_\infty}(B_i^2)$ is the Fourier transform of $P_\infty(/\underline{r} - \underline{r}'/)$. Hence A_i and H_i are given by

$$A_i = \overline{P}(B_i^2)E_i = \overline{P}(B_i^2) \sum_j (k_c \Sigma_{ac} \lambda_{ij} + k_b \Sigma_{ac} \nu_{ij}) C_j \tag{14}$$

$$H_i = \sum_n (p_c \lambda_{in} + p_b \nu_{in}) A_n$$

$$= \sum_n \overline{P}(B_n^2)(p_c \lambda_{in} + p_b \nu_{in}) \sum_j (k_c \Sigma_{ac} \lambda_{nj} + k_b \Sigma_{ab} \nu_{nj}) C_j \tag{15}$$

Substitution of the expansions (4) through (8) in the reactor equations and the linear independence of the $Z_i(\underline{r})$ requires

$$-D B_i^2 C_i - G_i + H_i = 0 \quad \text{for every i.} \tag{16}$$

In the manipulations given above we have solved for the G's and H's in terms of the C's. Hence, upon substitution of (9) and (14) in (16) we obtain an infinite set of linear homogeneous equations in the C's which is,

$$D B_i^2 C_i + \sum_j (\Sigma_{ac} \lambda_{ij} + \Sigma_{ab} \nu_{ij}) C_j$$

$$- \sum_j \sum_n \overline{P}(B_n^2)(p_c \lambda_{in} + p_b \nu_{in})(k_c \Sigma_{ac} \lambda_{nj} + k_b \Sigma_{ab} \nu_{nj}) C_j = 0 \tag{17}$$

The criticality condition is therefore the vanishing of the determinant of the coefficients of the C's.

In applications to be made to HRT, all absorption cross sections are expressed in terms of the pure moderator cross section, Σ_{ao}. Upon dividing each element of the critical determinant by Σ_{ao} one obtains,

$$\left| L_o^2 B_i \delta_{ij} + \left[(1 + w + z)\lambda_{ij} + \alpha \nu_{ij} \right] - \sum_n \bar{P}(B_n^2)(p_c \lambda_{in} + p_b \nu_{in})(\eta_c z \lambda_{nj} + k_b \alpha \nu_{nj}) \right| = 0 \qquad (18)$$

for the critical equation, where L_o^2 is the diffusion length of pure moderator (displacement of moderator is small), and z, w and α are core fuel, core poison and blanket absorption cross sections divided by Σ_{ao}.

$$Z_i(r) = \sqrt{\frac{2}{b}} \frac{1}{r} \sin \frac{i\pi r}{b} \qquad i = 1, 2, 3 \ldots \qquad (19)$$

then,

$$\nu_{ij} = \frac{1}{\pi} \left[\frac{\sin (i-j) \frac{\pi a}{b}}{i-j} - \frac{\sin (i+j) \frac{\pi a}{b}}{i+j} \right] \qquad (20)$$

and

$$\nu_{ij} = \delta_{ij} - \lambda_{ij} \qquad (21)$$

If there is no multiplication in the blanket (pure D_2O reflector) and no resonance capture in either the core or blanket, the summation over the index n in equation (18) reduces to a single term and the critical equation becomes,

$$\left| (L_o^2 B_i^2 + 1)\delta_{ij} + w \lambda_{ij} + (1 - \eta_c \bar{P}(B_i^2)\lambda_{ij} z \right| = 0 \qquad (22)$$

In this equation everything can be considered fixed except the concentration of fuel which is proportional to z. Hence, the problem is to solve equation (22) or, more generally, equation (18) for z.

A method of finding approximate solutions is indicated by the fact that the diffusion length in D_2O is very large and thus $L_o^2 B_i^2 \gg 1$ for all the D_2O moderated reactors of interest. For example, at 20°C $L_o^2 \simeq 10{,}000$ cm^2 and $L_o^2 B_i^2 > 1$ for reactor radii less than 314 cm. Hence, if we divide each row by $1 + L_o^2 B_i^2$, the elements of the determinant may be written in the form $\delta_{ij} + M_{ij}$, where M_{ij} falls off at least as fast as $1/i^3 j$. The n^{th} approximation to the root z is obtained by setting all the M_{ij} for $i > n$ and $j > n$ equal to zero. The infinite order determinant is thus in the n^{th} order approximation set equal to the $n \times n$ sub-determinant for which the M_{ij}'s have not been neglected. It should be noted that the fuel concentration is not involved in a transcendental way, but is obtained simply by the solution of an n^{th} degree algebraic equation. This method of approximation has turned out to be very convenient for calculating the HRT, since in this case one needs to consider only $n = 2$.

Tests of the Method and Comparison of Different Kernels

A series of test calculations were made for a Yukawa kernel, for which exact solutions can be obtained by the usual two-group analytical method. The results of these tests for a Yukawa kernel were then used to indicate the magnitude of the errors in the n^{th} approximation for a more general kernel such as the age-Yukawa.

The first series of calculations were made for two core radii and D_2O reflectors of several sizes. The basic data used are: $\eta = 2.09$, age in D_2O at 300°C equals 237 cm^2, $L_o^2 = 40{,}211$, $w = 0$ and $\alpha = 0$. The results in

terms of z, the ratio of fuel to pure moderator macroscopic absorption cross sections, are given in Table 1 for the various orders of approximation as defined above, where the subscript refers to the order of approximation. The exact two-group values for z are the z's having no subscript.

Table 1

Core Radius = 39 cm

Outer Reflector Radius (cm)	52	65	78	117
z	1424.55	434.32	281.40	175.80
z_1	1347.58	396.48	269.45	195.42
z_2	1369.35	422.96	276.96	175.02
z_3	1398.02	431.14	277.01	179.94
z_4	1416.43		279.88	
z_2/z	.961	.974	.984	.996
z_3/z	.981	.993	.984	1.024
z_4/z	.994		.995	

Core Radius = 78 cm

Outer Reflector Radius (cm)	104	130	630
z	57.79	41.02	24.70
z_1	57.71	42.23	153.17
z_2	57.64	40.96	63.39
z_3	57.76	40.98	41.40
z_2/z	.997	.998	2.566
z_3/z	.999	.999	1.676

These results show the convergence to be very rapid for all the cases where $L_0^2 B_i^2 \gg 1$; i.e., for all the outer radii less than about 600 cm. The only case of slow convergence, as is to be expected, is the one with the large reflector (630 cm radius).

As the reflector thickness is increased, the λ_{ij} tend to zero and the z obtained from any finite approximation to the determinant increase without limit.

The calculations were repeated for the 39 cm core radius using an age-Yukawa kernel with the same second moment as the single Yukawa and are recorded in Table 2. The "age" parameters in the age-Yukawa kernel were divided in the ratio 3:2 respectively.

Table 2

Age-Yukawa Kernel

	Outer Reflector Radius (cm)	65	78	117
	z_1	601.51	302.20	200.36
	z_2	708.01	370.40	192.25
	z_3	753.28	371.77	208.16
	z_4		381.03	
	z_2/z_1	1.18	1.23	.96
*Yukawa	z_2/z_1	1.07	1.03	.90
	z_3/z_2	1.06	1.00	1.08
Yukawa	z_3/z_2	1.02	1.00	1.03
	z_4/z_3		1.02	
Yukawa	z_4/z_3		1.01	

* The ratios of successive approximations obtained with a Yukawa kernel, Table 1.

Comparison of the ratios of successive approximations for the two kernels show the rate of convergence to be somewhat faster for the Yukawa kernel for the same reactor dimensions. However, since the Yukawa kernel predicts a much lower critical mass than does the age-Yukawa, comparison of rates of convergence should be made not for the same reactor dimensions but for equal z's. This point was not pursued further, since the results already indicate that the mathematical error in the z_2 approximation is probably less than 5 - 10% for reactors like the HRT.

The strong dependence of the critical mass on the slowing down kernel for small reactors is revealed in figure 1, in which is given the critical z predicted by the three standard kernels as a function of reflector thickness.

The applicability of the harmonics method to reactors with multiplication in a blanket was tested by comparing two-group calculations and z_2 harmonics approximations using a Yukawa kernel. The calculations were made for the HRT core with a blanket containing 300 grams of natural uranium in the form of UO_2SO_4 dissolved in D_2O. The results, given in Table 3, show the rate of convergence of the harmonics method to depend much more strongly on the blanket thickness than in the previous cases of pure D_2O reflector. The accuracy is, however, sufficient for HRT calculations.

The same calculations were repeated for a larger reactor having a core diameter of six feet and a blanket thickness of three feet, with disastrous results. Not only was the critical concentration predicted by the z_2 harmonics method in error by 50%, but the distribution of neutron absorptions and productions between core and reflector was completely erroneous. Although the critical mass of the larger D_2O reflected reactors can be calculated fairly

well with only two harmonics, they are, of course, not sufficient to give the detailed accuracy required for larger reactors having blankets with multiplication.

The authors record here their appreciation to T. Fowler who performed the computations with alacrity.

Table 3

Data

Core radius = 40.64 cm
Temperature = 280°C
Diffusion length of D_2O = 27,900 cm^2
Age of neutrons in D_2O = 212 cm^2
Multiplication constant in blanket = 0.899
Resonance escape probability in blanket = 0.730

	Reflector Thickness 67.73 cm			Reflector Thickness 81.28 cm			Reflector Thickness 101.60 cm		
	Two Group	Harmonics Method	% Error	Two Group	Harmonics Method	% Error	Two Group	Harmonics Method	% Error
Fast neutrons produced in core	.8275	.8318	+ .5	.6815	.6845	+ .4	.5163	.5257	+ 1.8
Fast neutrons produced in blanket	.1725	.1682	- 2.6	.3185	.3155	- .9	.4837	.4743	- 2.0
Thermal neutrons absorbed in core	.4058	.4053	- .1	.3368	.3458	+ 2.7	.2569	.2766	+ 7.7
Thermal neutrons absorbed in blanket	.1401	.1357	- 3.1	.2586	.2619	+ 1.3	.3928	.4085	+ 4.0
Resonance neutrons absorbed in blanket	.0822	.0843	+ 2.3	.1187	.1401	+18.0	.1570	.2017	+28.5
Fast neutron leakage	.2176	.2272	+ 4.4	.1513	.1122	-25.8	.0980	.0225	-78.0
Slow neutron leakage	.1546	.1475	- 4.6	.1348	.1399	+ 3.8	.0954	.0907	- 4.9
z	288	289.57	+ .5	217.2	219.27	+ 1.0	179.0	192.98	+ 7.8
Thermal neutrons absorbed in U-238	.0802	.0777	- 3.1	.1480	.1499	+ 1.3	.2248	.2338	+ 4.0
Thermal neutrons absorbed in U-235 in core	.3960	.3955	- .1	.3261	.3334	+ 2.2	.2470	.2667	+ 8.0
Thermal neutrons absorbed in U-235 in blanket	.0825	.0800	- 3.0	.1524	.1537	+ .9	.2314	.2406	+ 4.0
Thermal neutrons absorbed in U-235 total	.4785	.4755	- .6	.4785	.4871	+ 1.8	.4784	.5073	+ 6.0
Plutonium produced	.1624	.1620	- .2	.2667	.2900	+ 8.7	.3818	.4355	+14.1
Core conversion ratio	.4101	.4096	- .1	.8178	.8698	+ 6.4	1.6500	1.8101	+ 9.7
Total conversion ratio	.3390	.3407	+ .5	.5574	.5954	+ 6.8	.7981	.8585	+ 7.6